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Reformulating Real-time Optimal Feedback based on Model Uncertainty

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Abstract:
Model Predictive Control (MPC) and its first order approximation, the Neighboring Extremals (NE) have been used for real-time optimal control in the presence of model uncertainties for several decades. Traditionally, both MPC and NE would only correct for deviations in states considering the underlying model to be nominal - a procedure that is valid for additive disturbances. However, in the presence of model uncertainties, a simple illustrative example in this paper shows that such a MPC scheme or a NE controller could cause corrections in the wrong direction, thereby deteriorating performance. The paper, thus, addresses reformulating NE feedback considering sensitivities with respect to the model parameters. The feedback then has two components - one based on state deviations and the other based on parameter deviations. Note that this formulation also requires some primitive form of parameter estimation. The illustrative example shows the efficacy of this approach and the importance of incorporating the knowledge of parameter variations in real-time optimal control.

Keywords: Neighboring Extremal; Model Predictive Controller; Necessary Conditions of Optimality; Parametric Uncertainty

1. INTRODUCTION

Real-time optimal control of batch processes under the presence of model uncertainty has been posing as an invincible challenge to the control community. Traditionally, open-loop optimal trajectory based on a nominal offline model is employed for control of batch processes. In the presence of uncertainties, robust optimal trajectory that minimizes either the worst case deviation of the batch-end performance index or the variance of the objective around the nominal value (caused by the uncertainty in the parameters) is used (Nagy and Braatz, 2004). Also, run-to-run adaption strategies with repetitive identification of the uncertain parameters towards the end of the batch have been developed in the literature (Lee and Lee, 2007, 2003).

With the advent of the Model Predictive Control (MPC) real-time optimal control by repetitive optimization of the dynamic formulation is made possible. The MPC formulation uses a nominal model along with state feedback in order to find the future optimal input moves (Eaton and Rawlings, 1990). Even though, MPC is a proven technology in process industries, the huge computation cost involved in solving the formulation can make it formidably unattractive for the control of batch processes. Thus, measurement based optimization schemes that track the NCO have been developed (Srinivasan et al., 2003), which characterize the nominal solution using boundary and interior arcs, apply simple constraint-tracking techniques for the boundary arcs and use suitable approximations for the interior arcs. The current study, explores the NCO tracking based controller for the interior arcs by designing a Neighboring Extremal (NE) Controller. NE controller is a first-order approximation of the MPC where the deviation of the input is obtained from the deviation of the states (Bryson and Ho, 1969). It is a computationally efficient solution for small variations and for processes that are not heavily nonlinear.

Traditionally, the nominal model is used as a basis for designing both MPC and NE controller. Parameters of the model are typically not adapted due to the absence of persistency of excitation and the corrective actions for the input are based only on the state deviations. Such an approach is valid in the presence of additive uncertainty, *i.e.,* state and process noise. However, when state deviations are caused by model uncertainties, the correction should depend not only the state deviations (the effect), but also on the model uncertainties (the cause). So, the objective of the paper is to emphasize the importance of incorporating the model uncertainty information in the correction. Incorporating model uncertainty information in the MPC based control strategy needs prudence, since adapted parameter values with poor confidence would cause the input to chatter. So, a safer bet would be to use the NE feedback law that incorporates corrections based on both state and parameter variations.

2. MODEL PREDICTIVE CONTROL VS NCO-TRACKING BASED CONTROL

2.1 MPC formulation

Design of Model Predictive Control for batch processes, typically involves repetitive optimization based on an offline model and the necessary states information obtained from the measurements (Chin et al., 2000). Considering the state feedback at time, t_k to be x_k, an optimization problem is formulated as follows,

$$\min_{u[t_k,t_f]} J = \Phi(x(t_f)) + \int_{t_k}^{t_f} L(x(t), u(t))\, dt \tag{1}$$

$$\text{s.t} \qquad \dot{x}(t) = F(x(t), u(t)), \quad x(t_k) = x_k \tag{2}$$

where t_f is the batch time, $\Phi(x(t_f))$ is the terminal cost function and L is the integral cost function, while J is the cost function to be minimized. x is the state vector with the initial conditions for solving state equations from time t_k to t_f as x_k and F describes the system dynamics. However, instead of this scheme that requires the explicit solution of the above formulation at each sampling time, Measurement Based Optimization (MBO) schemes have been developed in the literature (Welz et al., 2008; Gros et al., 2009a,b). One among such approaches is the NCO-based tracking control, which can be understood as a first order (linear) approximation of the MPC formulation.

2.2 Necessary conditions of optimality

Consider the formulation of the unconstrained optimal control problem as follows,

$$\min_{u[0,t_f]} J = \Phi(x(t_f)) + \int_{0}^{t_f} L(x(t), u(t))\, dt \tag{3}$$

$$\text{s.t} \qquad \dot{x}(t) = F(x(t), u(t)), \quad x(0) = x_0 \tag{4}$$

Furthermore, assuming that if all the functions in Eqs. (3) and (4) are continuously differentiable with respect to their arguments, then there exists optimal control $u^*(t)\, \forall t$, $0 \le t \le t_f$ for the nominal parameter values. Note that this solution profile consists of only interior (sensitivity-seeking) arc. Furthermore, in order to be operated in an optimal fashion, the NCO are tracked *.i.e.,* first order partial derivatives of the Hamiltonian function with respect to the input profile must always be zero, at any given time.

Based on Pontryagin's Minimum Principle (PMP), the problem of optimizing the scalar cost functional J in Eqs. (3) and (4) can be reformulated by defining the Hamiltonian function $H(t)$ as (Bryson and Ho, 1969):

$$H(x, u, \lambda) = L(x, u) + F(x, u)^{\mathrm{T}} \lambda \tag{5}$$

and the necessary conditions of optimality give

$$H_u = L_u + {F_u}^{\mathrm{T}} \lambda = 0\,; \quad H_{uu} > 0\,, \tag{6}$$

where λ represents the adjoint vector function given as

$$\dot{\lambda} = -H_x = -L_x - {F_x}^{\mathrm{T}} \lambda\,; \quad \lambda(t_f) = \Phi_x(x(t_f)) \tag{7}$$

Therefore, the solution of Eq. (6) gives the optimal input profile even in the presence of process disturbances and uncertainties. During the implementation of the NCO tracking based control, boundary arcs can be easily tracked. However, in order to push the path sensitivities to zero, approximate methods such as neighboring extremal control must be employed (Gros et al., 2009b).

2.3 Design of neighboring extremal controller for non-singular systems

As the optimal control profile $u^*(t)$, $0 \le t \le t_f$ is designed based on the initial condition x_0, any slight variation δx_0 in the initial states requires the modification of the entire profile. For the case of unconstrained problems or when the constraints remain inactive, the first-order approximation of the optimal trajectory for the perturbed control is considered as

$$u(t;\eta) = u^*(t) + \eta \delta u(t) + o(\eta) \tag{8}$$

and the correction δu is computed as the solution of the so-called *accessory minimum problem*, *.i.e.*, the minimization of the second-order variation of the cost functional subject to the linearized dynamics (Breakwell et al., 1963),

$$\min_{\delta u(t)} \delta^2 J = \frac{1}{2} \delta x(t_f)^{\mathrm{T}} \Phi^*_{xx} (\delta x(t_f)) + \frac{1}{2} \int_0^{t_f} \begin{pmatrix} \delta x \\ \delta u \end{pmatrix}^{\mathrm{T}} \begin{pmatrix} H^*_{xx} & H^*_{xu} \\ H^*_{ux} & H^*_{uu} \end{pmatrix} \begin{pmatrix} \delta x \\ \delta u \end{pmatrix} dt \tag{9}$$

$$\text{s.t} \qquad \delta \dot{x}(t) = F^*_x \delta x + F^*_u \delta u, \quad \delta x(0) = \delta x_0 \tag{10}$$

Thus, when the problem of (9) and (10) has a solution, it can be shown that there exists an optimal control trajectory $u(t;\eta)$, in the neighborhood of $\eta = 0$. Therefore, the correction δu satisfying the strengthened Legendre-Clebsch condition $H^*_{uu}(t) > 0$ along the nominal solution $u^*(t), x^*(t), \lambda^*(t)$, is then given by

$$\delta u(t) = -(H^*_{uu})^{-1} [H^*_{ux} \delta x(t) + {F^*_u}^{\mathrm{T}} \delta \lambda] \tag{11}$$

Furthermore, a NE state feedback law that enforces the necessary conditions of optimality can be designed via backward sweep method that assumes linear relation between the states and adjoint variables as $\delta\lambda(t) = S_x(t)\delta x(t)$ (Gros et al., 2009b).

$$\delta u(t) = -K_x \delta x(t) \tag{12}$$

$$K_x(t) = (H^*_{uu})^{-1} (H^*_{ux} + F^{*\mathrm{T}}_u S_x(t)) \tag{13}$$

$$\dot{S}_x(t) = -H^*_{xx} - S_x(t) F^*_x - F^{*\mathrm{T}}_x S_x(t) + (H^*_{xu} + S_x(t) F^*_u) K_x(t)\,; \text{with } S_x(t_f) = \Phi^*_{xx} \tag{14}$$

3. NEIGHBORING EXTREMAL CONTROL IN THE PRESENCE OF MODEL UNCERTAINTIES

3.1 Reformulation of neighboring extremal feedback in the presence of model uncertainties

In the presence of model uncertainties, the unconstrained optimal control problem as described using Eqs. (3) and (4), can be reformulated as follows:

$$\min_{u(t)} J = \Phi(x(t_f)) + \int_{0}^{t_f} L(x(t), u(t), \theta)\, dt \tag{15}$$

$$\text{s.t} \qquad \dot{x}(t) = F(x(t), u(t), \theta), \quad x(0) = x_0 \tag{16}$$

The Hamiltonian function $H(t)$ for the above formulation can thus be derived as,

$$H(x, u, \theta, \lambda) = L(x, u, \theta) + F(x, u, \theta)^{\mathrm{T}} \lambda \tag{17}$$

while the *accessory minimum problem* will be,

$$\min_{\delta u(t)} \delta^2 J = \frac{1}{2}\delta x(t_f)^{\mathrm{T}}\Phi^*_{xx}(\delta x(t_f)) + \frac{1}{2}\int_0^{t_f} \begin{pmatrix}\delta x\\ \delta u\\ \delta\theta\end{pmatrix}^{\mathrm{T}} \begin{pmatrix} H^*_{xx} & H^*_{xu} & H^*_{x\theta}\\ H^*_{ux} & H^*_{uu} & H^*_{u\theta}\\ H^*_{\theta x} & H^*_{\theta u} & H^*_{\theta\theta}\end{pmatrix} \begin{pmatrix}\delta x\\ \delta u\\ \delta\theta\end{pmatrix} dt \quad (18)$$

$$\text{s.t} \qquad \delta\dot{x}(t) = F^*_x\delta x + F^*_u\delta u + F^*_\theta\delta\theta, \quad \delta x(0) = \delta x_0 \quad (19)$$

Thus, when the problem of (18) and (19) has a solution, it can be shown that there exists an optimal control trajectory $u(t;\eta)$, in the neighborhood of $\eta = 0$. Therefore, the correction δu satisfying the strengthened Legendre-Clebsch condition $H^*_{uu}(t) > 0$ condition along the nominal solution $u^*(t), x^*(t), \lambda^*(t)$, is then given by

$$\delta u(t) = -(H^*_{uu})^{-1}[H^*_{ux}\delta x(t) + {F^*_u}^{\mathrm{T}}\delta\lambda + H^*_{u\theta}\delta\theta] \quad (20)$$

Furthermore, by assuming a linear relationship as $\delta\lambda(t) = S_x(t)\delta x(t) + S_\theta(t)\delta\theta$ (Gros et al., 2009b).

$$\delta u(t) = -K_x\delta x(t) - K_\theta\delta\theta \quad (21)$$

$$K_x(t) = (H^*_{uu})^{-1}(H^*_{ux} + {F^*_u}^{\mathrm{T}}S_x(t)) \quad (22)$$

$$K_\theta(t) = (H^*_{uu})^{-1}(H^*_{u\theta} + {F^*_u}^{\mathrm{T}}S_\theta(t)) \quad (23)$$

$$\dot{S}_x(t) = -H^*_{xx} - S_x(t)F^*_x - {F^*_x}^{\mathrm{T}}S_x(t) + (H^*_{xu} + S_x(t)F^*_u)K_x(t)\,; \text{with } S_x(t_f) = \Phi^*_{xx} \quad (24)$$

$$\dot{S}_\theta(t) = -H^*_{x\theta} - S_x(t)F^*_\theta - {F^*_x}^{\mathrm{T}}S_\theta(t) + (H^*_{xu} + S_x(t)F^*_u)K_\theta(t)\,; \text{with } S_\theta(t_f) = 0 \quad (25)$$

Remark: The gains of the neighboring extremal controller, K_x and K_θ, are obtained by solving the Riccati equation within the unconstrained arcs. However, in cases where the analytical expression for the nominal input trajectory, $u^*(t)$, is known, the above procedure can be avoided. Instead, as the gains represent the input sensitivities to the states and model parameters, they can be derived as,

$$K_x(t) = -\frac{\partial u^*}{\partial x} \quad (26)$$

$$K_\theta(t) = -\frac{\partial u^*}{\partial \theta} \quad (27)$$

Although, the reformulated NE feedback incorporates the input sensitivities with respect to the model parameters, the information regarding the deviations in the model parameters is not readily available. Hence, methods for parameter identification based on online state feedback have to be incorporated into this framework.

3.2 Online estimation of deviations in model parameters from state feedback

In the case of steady state processes, it has been shown that the deviations in model parameters can be estimated via output feedback (Gros et al., 2009a). On the other hand, in the case of unsteady state processes, this can be done only when reliable methods for estimating the derivative component are available. The equation governing the system is described as,

$$\dot{x} = F(x, u, \theta), \quad x(0) = x_0 \quad (28)$$

where x and F represent the states and state dynamics, respectively. u is the input and θ represents the model parameters. Consider process operation around a nominal operating trajectories, $\dot{x}^* = F(x^*, u^*, \theta_{nom})$ and a perturbation is made in the model parameters, $\delta\theta = \theta - \theta_{nom}$ from the nominal parameters. Let $\delta u_k = u_k - u^*_k$ be the corrective action made at each instant in order to be at the optimality. Thus, the deviations from θ_{nom} and u^*_k induce change in the system states as, $\delta x_k = x_k - x^*_k$. Hence, the linearization around the nominal operating trajectories results in,

$$\delta\dot{x}_k = F_x\delta x_k + F_u\delta u_k + F_\theta\delta\theta, \quad \forall k \quad (29)$$

Thus, based on the state feedback, the deviations in the model parameters are estimated as,

$$\delta\theta = F^\dagger_\theta(\delta\dot{x}_k - F_x\delta x_k - F_u\delta u_k) \quad (30)$$

However, the limitation concerning the online estimation of $\delta\dot{x}_k$ due to the causality issues, in both discrete and continuous time, discourages its further implementation.

Alternatively, an integral approach is employed in this study, for online estimation of the deviations in model parameters based on state feedback. Using the nominal model along with the values of the current inputs and states, the future state values are predicted as,

$$\dot{\hat{x}} = F(x, u, \theta_{nom}) - \gamma(\hat{x} - x); \quad \hat{x}(k) = x_k \quad (31)$$

Here, as the current states and inputs are used, the linearized model can be represented as,

$$\delta\dot{\hat{x}} = \dot{\hat{x}} - \dot{x} = -F_\theta\delta\theta - \gamma(\hat{x} - x); \quad \delta\hat{x}(k) = 0 \quad (32)$$

where γ acts as a filter avoiding the integral to become too large. Besides, it also acts as a forgetting factor for the predicted states. In order to estimate the deviations in the model parameters using the state feedback, the sensitivity of the $\delta\hat{x}$ with respect to θ at each instant, M_k, have to be computed. Thus,

$$\frac{\partial(\delta\dot{\hat{x}})}{\partial\theta} = \frac{\partial(\dot{\hat{x}} - \dot{x})}{\partial\theta} = \dot{M} = -F_\theta - \gamma M; \quad M(0) = 0 \quad (33)$$

$$\delta\theta = M^\dagger_k(\hat{x}_k - x_k), \forall k \quad (34)$$

By simultaneously solving the coupled equations *.i.e.*, Eqs. (31) and (33), the deviations in the model parameters can be repeatedly estimated based on Eq. (34). Furthermore, in order to avoid the issue concerning the inversion of $M(0) = 0$ in Eq. (34), we can use $M(0) = -1$. Also, by choosing the value of γ sufficiently large, the effect of choosing a non-zero initial condition for solving the sensitivity equations is damped over time.

4. ILLUSTRATIVE EXAMPLE

4.1 Process model

The isomerization reaction system $A \leftrightarrow B$ in a batch chemical reactor is considered in this study. This example represents a non-input-affine system and thus serves as non-singular system. Species A is initially present in the reactor and B is the desired product. A simple dynamical model is derived for the system based on mass-balance principles as,

$$\dot{c_A} = -k_1c_A + k_2(c_{A,0} - c_A), \quad c_A(0) = c_{A,0} \quad (35)$$

where c_A represents the concentration [mol L^{-1}] of species A, k_1 and k_2 are the kinetic coefficients [hr^{-1}] and $c_{A,0}$ is the initial condition. As there are no additional species, the concentration of species B will be, $c_B = c_{A,0} - c_A$. The

Table 1 Parameters used in the model

Parameter	Symbol	Value	Units
Initial concentration	$c_{A,0}$	5	mol L^{-1}
Batch time	t_f	1	hr
Kinetic parameters	$k_{1,0}$	5×10^3	hr^{-1}
	$k_{2,0}$	7×10^{16}	hr^{-1}
	E_1	2×10^4	J mol^{-1}
	E_2	1×10^5	J mol^{-1}
	$\bar{k}_{1,0}$	1	–
	$\bar{k}_{2,0}$	0.0224	–
	α	5	–
Gas constant	R	8.314	J mol^{-1} K^{-1}

kinetic coefficients are represented using an Arrhenius type equation as,

$$k_i = k_{i,0} \exp\left(-\frac{E_i}{RT}\right), \quad \text{where, } i = 1, 2. \tag{36}$$

By considering $\alpha = E_2/E_1$, the equations for the kinetic coefficients are further scaled as,

$$k_1 = \bar{k}_{1,0}u \quad \text{and} \quad k_2 = \bar{k}_{2,0}u^\alpha \tag{37}$$

$$\text{where} \quad u = k_{1,0} \exp\left(-\frac{E_1}{RT}\right) \tag{38}$$

$$\bar{k}_{1,0} = 1 \quad \text{and} \quad \bar{k}_{2,0} = k_{2,0}\left(\frac{1}{k_{1,0}}\right)^\alpha \tag{39}$$

With an objective to maximize the conversion of species A, the optimal control problem can thus be formulated as:

$$\min_{u(t)} J = \Phi(x(t_f)) = -\left(1 - \frac{c_A}{c_{A,0}}\right)\Bigg|_{t_f} \tag{40}$$

where t_f represents the final batch time. The nominal values of the parameters used in the above model expressions are provided in Table 1.

4.2 Characterization of the nominal solution

As presented in Eqs. (35) - (40), the open-loop optimal control problem is unconstrained. Thus, the Necessary Conditions of Optimality according to Eq. (6) must hold good and hence,

$$H_u = \lambda(-\bar{k}_{1,0}c_A + \bar{k}_{2,0}(c_{A,0} - c_A)\alpha u^{\alpha-1}) = 0 \tag{41}$$

Thus, the analytical solution for the optimal input trajectory, $u^*(t)$, is obtained as,

$$u^* = \left(\frac{\bar{k}_{1,0}c_A}{\bar{k}_{2,0}(c_{A,0} - c_A)\alpha}\right)^{\left(\frac{1}{\alpha-1}\right)} \tag{42}$$

4.3 Design of neighboring extremal controller

The Neighboring Extremal Controller makes use of the information regarding the deviations in the states and model parameters (uncertainty) from their corresponding nominal values, in order to make a corrective action to the input from the nominal trajectory. For designing the NE controller, the only state $x = c_A$ is assumed to be measurable. As the system has only one state (or measurement), parametric uncertainties existing in more than one parameter cannot be obtained, due to rank deficiency. Hence, perturbations in the parameters, $\theta = [\bar{k}_{1,0}, \bar{k}_{2,0}, \alpha]$, are considered individually, but not expected to occur simultaneously. In this example, as the analytical expression for the input trajectory is known, the NE controller gains can be derived based on Eqs. (26) - (27).

$$K_x = -\frac{c_{A,0}u^*}{c_A(\alpha-1)(c_{A,0} - c_A)} \tag{43}$$

$$K_{\theta_1} = -\frac{u^*}{(\alpha-1)\bar{k}_{1,0}} \tag{44}$$

$$K_{\theta_2} = \frac{u^*}{(\alpha-1)\bar{k}_{2,0}} \tag{45}$$

$$K_{\theta_3} = \frac{u^*}{(\alpha-1)}\left(log(u^*) + \frac{1}{\alpha}\right) \tag{46}$$

These analytical expressions can also be derived from Eq. (20) using the higher order partial derivatives of the Hamiltonian function $H(t)$.

4.4 Results and discussions

By considering various scenarios of uncertainties in model parameters, a comparative study on the performance of different versions of NE controller is carried out.

$$\bar{k}'_{1,0} = \bar{k}_{1,0}(1 + \Delta\theta_1) \tag{47}$$

$$\bar{k}'_{2,0} = \bar{k}_{2,0}(1 + \Delta\theta_2) \tag{48}$$

$$\alpha' = \alpha(1 + \Delta\theta_3) \tag{49}$$

where $\Delta\theta_1$ and $\Delta\theta_2$ are the uncertainties in the scaled kinetic coefficients $\bar{k}_{1,0}$ and $\bar{k}_{2,0}$, respectively, while $\Delta\theta_3$ is the uncertainty in α. Thus, $\Delta\theta_i = 0$, $i = 1, 2$ and 3, represent the nominal parameters. The focus of this study is to understand the effect of each of the gains on the corrective action made in the input trajectory and thus, its consequence on the product quality values. Hence, for comparison, the information regarding the state, c_A and the uncertainty in the model parameter, $\Delta\theta_i$ are assumed to be precisely known. Different case studies as given in Table 2 were considered during this study.

During the implementation, three different versions of the NE controller are considered depending on the feedback available. The first among them is the traditional NE controller with (i) only K_x with δx feedback (NE-δx). Assuming that the deviations in the parameters are precisely known, NE controller gain corresponding to input sensitivity with respect to the parameters, K_θ is kept active along with K_x. Thus, the second version of the NE controller with (ii) both K_x and K_θ with δx and *known* $\delta\theta$ feedback (NE-δx-$\delta\theta$) is considered during this study in order to account for the optimality loss that can be recovered with the inclusion of K_θ. However, as $\delta\theta$ values are not readily availables, the estimated deviations in the parameters ($\delta\theta_{pred}$) are obtained using a repetitive estimation method (as discussed in Section 3.2) by choosing $\gamma = 100$. Thus, the results obtained through the implementation of NE controller with (iii) both K_x and K_θ with δx and *estimated* $\delta\theta_{pred}$ feedback (NE-δx-$\delta\theta_{pred}$) is also included. Additionally, two versions of the MPC formulation (iv) with only δx feedback (MPC-δx) and

(v) with both δx and *estimated* $\delta\theta_{pred}$ feedback (MPC-δx-$\delta\theta_{pred}$) are included for this comparative study. Not to mention, the version of MPC that requires the feedback of both δx and *known* $\delta\theta$ gives the results corresponding to the *true* optimal solution.

Figures 1(a) represents the input profiles resulting from the implementation of all the three versions of the NE controller along with the two versions of the MPC formulation for Case 1. For comparison, assuming that the uncertainty is precisely known the true optimal input profile for Case 1 is also provided. Besides, the nominal input profile is also shown in the plot as it serves as a benchmark to realize the performance of both NE controller and MPC formulation. With all the profiles being very close to each other, a part of the plot is magnified for a better view (in the inset). As can be seen from the plots, the traditional NE controller with only K_x gain and δx feedback (NE-δx) and the the MPC formulation with only δx state feedback (MPC-δx) make corrective actions to the nominal input towards a wrong direction. On the other, the NE-δx-$\delta\theta$ seeks the correct direction, however, leads to over-compensation for the perturbation introduced. Towards this end, model parameter is identified very well as shown in Figure 1(b). Thus, NE-δx-$\delta\theta_{pred}$ provides the corrective actions that track an input profile that is closer to NE-δx-$\delta\theta$. While, in the case of MPC-δx-$\delta\theta_{pred}$, the input profile moves towards the right direction and reaches very close to the *true* optimal profile. Thus, in the presence of model uncertainties, the true potential of NE controller and MPC formulation is realized when they are designed in a full fledged fashion incorporating the deviations in both states and model parameters.

Also, Figures 2(a) and 3(a) provide the input profiles for cases 2 and 3, respectively, that infer similar trends in the performance of the different versions of the controller. The product quality values obtained towards the end of the batch for each of the case studies are provided in Table 3. Clearly, NE-δx-$\delta\theta$ outperforms the rest of them by resulting in better product quality values. The versions NE-δx-$\delta\theta_{pred}$ and MPC-δx-$\delta\theta_{pred}$ try to drive the process closer to the *true* optimal. On the other hand, NE-δx and MPC-δx, compete only in being either close to or worse than the open-loop nominal performance. Thus, the important message to be conveyed through this exercise is that, in the presence of model uncertainties, the MPC formulation that does not incorporate the deviations in the model parameters (or, which does not update the model) shows a performance that is not even to the level that is delivered by implementing the nominal open loop profile. The same accounts even for the NE-δx controller. However, in certain cases, like in Case 2, as the NE controller is a first order approximation of the MPC, the corrective actions made by it does not make the input profile deviate as largely as observed in the case of MPC-δx. This can be seen in Figures 2(a).

Therefore, this discussion leads us to the most important insight of incorporating the model parameter deviations along with the state feedback during real-time optimal control of batch processes. Precisely, as discussed in the literature (Eaton and Rawlings, 1990; Agarwal, 1997)), robust control and real-time optimal operation is possible when online re-estimation of the model parameters or their deviations from the nominal values is enabled along with the state feedback. Hence, in the presence of uncertainty, repetitive online optimization based only on the state feedback may be futile.

From the plots in Figures 1(b) and 3(b), it can be inferred that repetitive estimation of the parameters for this illustrative example performs well for both NE-δx-$\delta\theta_{pred}$ and MPC-δx-$\delta\theta_{pred}$. However, in Case 2 as seen in Figure 2(b), the issue concerning the simultaneous control and parameter estimation during real time control of batch process poses as a hurdle to identify the level of deviations in the parameters.

5. CONCLUSIONS

Real-time optimal control in the presence of model uncertainties is demonstrated using the Neighboring Extremal controller. The importance of considering the input sensitivities with respect to the model parameters, apart from its sensitivities to the states is the major focus of this study. With the help of a simple illustrative example, it has been shown that NE controller with both K_x and K_θ gains (NE-δx-$\delta\theta$) shows a better performance overall. In fact, the input and state trajectories corresponding to the NE-δx-$\delta\theta$ version track the *true* optimal profiles very closely. Hence, the necessity and the importance of reformulating the NE feedback to counter the deviations in the model parameters has been addressed in this study. Furthermore, these conclusive remarks also provide the evidence to prove the limitation of online reoptimization control technologies, like Model Predictive Control, whose corrective actions are made based on predictions of the nominal model along with online state feedback. Thus, it has to be noted that these control strategies are useful only in the presence of deviations in the initial states, but fail to achieve the performance in the presence of deviations in the model parameters. Evidence from the earlier literature also stands in support of our statements (Agarwal, 1997).

REFERENCES

M. Agarwal. Feasibility of on-line reoptimization in batch processes. *Chemical Engineering Communications*, 158 (1):19–29, 1997.

J. Breakwell, J. Speyer, and A. Bryson. Optimization and control of nonlinear systems using the second variation. *Journal of the Society for Industrial and Applied Mathematics Series A Control*, 1(2):193–223, 1963.

A.E. Bryson and Y.C. Ho. *Applied optimal control: optimization, estimation, and control.* Blaisdell book in the pure and applied sciences. Blaisdell Pub. Co., 1969.

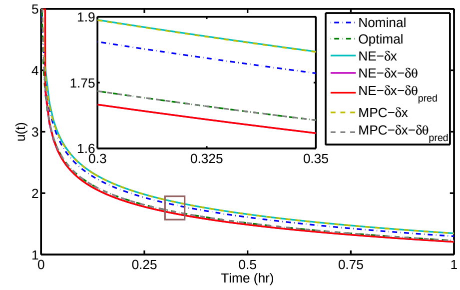
In S. Chin, Kwang S. Lee, and Jay H. Lee. A technique for integrated quality control, profile control, and constraint handling for batch processes. *Industrial & Engineering Chemistry Research*, 39(3):693–705, 2000.

J.W. Eaton and J.B. Rawlings. Feedback control of chemical processes using on-line optimization techniques. *Computers & Chemical Engineering*, 14(4-5):469–479, 1990.

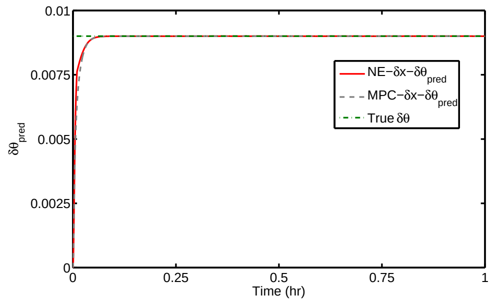
S. Gros, B. Srinivasan, and D. Bonvin. Optimizing control based on output feedback. *Computers & Chemical Engineering*, 33(1):191–198, 2009a.

Table 2 Product quality values (in conversion) for different cases

Case	Perturbations in model parameters			True optimal	Nominal profile	NCO tracking controller			MPC formulation	
	$\Delta\theta_1$	$\Delta\theta_2$	$\Delta\theta_3$			NE-δx	NE-δx-$\delta\theta$	NE-δx-$\delta\theta_{pred}$	MPC-δx	MPC-δx-$\delta\theta_{pred}$
Nominal	0.0	0.0	0.0	0.7581	0.7581	0.7581	0.7581	0.7581	0.7581	0.7581
1	0.0	0.4	0.0	0.7367	0.7342	0.7309	0.7362	0.7362	0.7312	0.7367
2	0.0	0.0	0.2	0.7299	0.7184	0.6931	0.7267	0.7228	0.4252	0.7270
3	0.2	0.0	0.0	0.8126	0.8123	0.8113	0.8124	0.8119	0.8115	0.8120



(a) Input profiles



(b) $\delta\theta$ estimates

Fig. 1 Case 1, with perturbations only in $\bar{k}_{2,0}$.

S. Gros, B. Srinivasan, B. Chachuat, and D. Bonvin. Neighbouring-extremal control for singular dynamic optimisation problems. Part I: single-input systems. *International Journal of Control*, 82:1099–1112, 2009b.

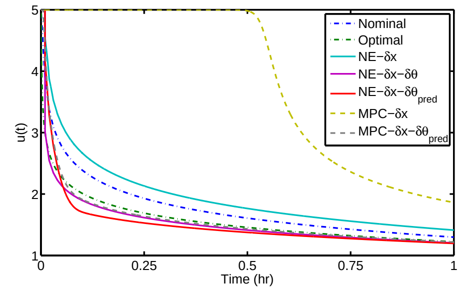
J. H. Lee and K. S. Lee. Iterative learning control applied to batch processes: An overview. *Control Engineering Practice*, 15(10):1306–1318, 2007.

Kwang S. Lee and Jay H. Lee. Iterative learning control-based batch process control technique for integrated control of end product properties and transient profiles of process variables. *Journal of Process Control*, 13(7): 607–621, 2003.

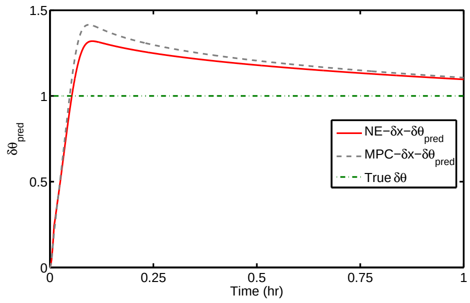
Z. K. Nagy and R. D. Braatz. Open-loop and closed-loop robust optimal control of batch processes using distributional and worst-case analysis. *Journal of Process Control*, 14(4):411–422, 2004.

B. Srinivasan, D. Bonvin, E. Visser, and S. Palanki. Dynamic optimization of batch processes II. Role of measurements in handling uncertainty. *Computers & Chemical Engineering*, 27(5):761–761, 2003.

C. Welz, B. Srinivasan, and D. Bonvin. Measurement-based optimization of batch processes: Meeting terminal constraints on-line via trajectory following. *Journal of Process Control*, 18(34):375 – 382, 2008.

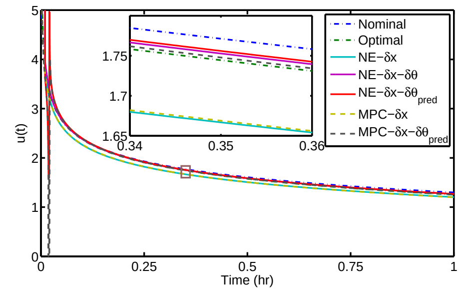


(a) Input profiles

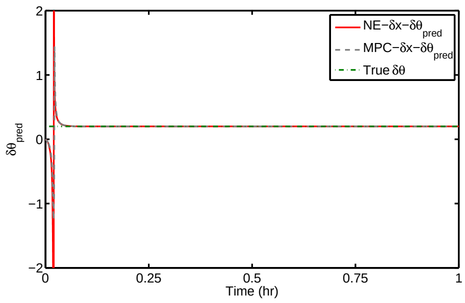


(b) $\delta\theta$ estimates

Fig. 2 Case 2, with perturbations only in α.



(a) Input profiles



(b) $\delta\theta$ estimates

Fig. 3 Case 3, with perturbations only in $\bar{k}_{1,0}$.